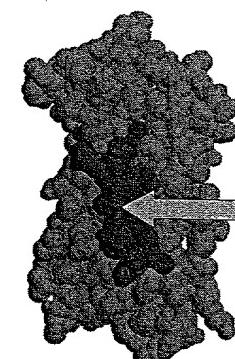


Fig. 1

The Principle of Ligand Identification

The Process



Goal: Identification of a ligand that binds to a predefined protein surface area (active site)

Dissection of the protein surface in molecular surface patches (MSPs)



Definition of MSP(s) forming the active site for which a ligand has to be identified

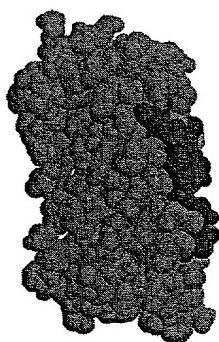
Search for MSPs (basis patches) in the databank that are similar to the active site MSP(s) with respect to geometric parameters and fitting atomic species



The contact patch is supposed to be complementary to the active site MSP.

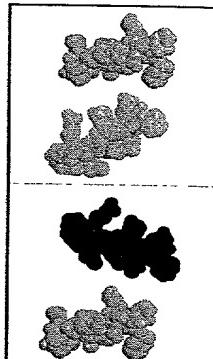


Transformation of co-ordinates of the contact patch-SSEs on the active site MSP and evaluation of the fit by local atomic density [3].

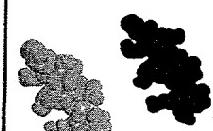


Abbreviations:
SSE: secondary structural element
MSP: molecular surface patch

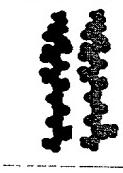
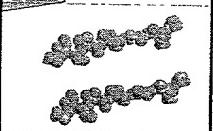
Dictionary of Interfaces in Proteins



SSE with basis patch



SSE with contact patch



The „Dictionary of Interfaces in Proteins“ (DIP) is a collection of interfaces that are defined as pairs of matching molecular surface patches between neighboring secondary structural elements. Each interface consists of two subsets of atoms from neighbouring secondary structure elements (pairs of complementary MSPs). All such interfaces from known protein structures were collected in a comprehensive data bank (DIP).

Figure 2